d his

L1   450 S (PROTEIN (5W)((X(2W)RAY) OR CRYSTAL?)) AND (MOLECULAR REPLACE
L2   71 S L1 AND (SEARCH MODEL)

=> d bib, abs 19,24,25

L2   ANSWER 19 OF 71 CAPLUS COPYRIGHT 2004 ACS on STN
AN   2001:695651 CAPLUS
DN   135:368799
TI   How to take advantage of non-crystallographic symmetry in
      molecular replacement: 'locked' rotation and translation
      functions
AU   Tong, Liang
CS   Department of Biological Sciences, Columbia University, New York, NY,
      10027, USA
SO   Acta Crystallographica, Section D: Biological Crystallography (2001),
      D57(10), 1383-1389
      CODEN: ABCRE6; ISSN: 0907-4449
PB   Munksgaard International Publishers Ltd.
DT   Journal
LA   English
AB   Many protein mols. form assemblies that obey point-group symmetry. These
      assemblies are often situated at general positions in the unit cell such
      that the point-group symmetry of the assembly becomes non-crystallog.
      symmetry (NCS) in the crystal. The presence of NCS places significant
      constraints on structure determination by the **mol.-replacement**
      method. The locked rotation and translation functions have been developed
      to take advantage of the presence of NCS in this structure determination, which
      generally requires four steps. (i) The locked self-rotation function is
      used to determine the orientation of the NCS assembly in the crystal, relative
      to a pre-defined 'standard' orientation of this NCS point group. (ii) The
      locked cross-rotation function is used to determine the orientation of one
      monomer of the assembly in the standard orientation. This calcn. requires
      only the structure of the monomer as the **search model**.
      (iii) The locked translation function is used to determine the position of this
      monomer relative to the center of the assembly. Information obtained from
      steps (ii) and (iii) will produce a model of the entire assembly centered
      at the origin of the coordinate system. (iv) An ordinary translation
      function is used to determine the center of the assembly in the crystal unit
      cell, using as the **search model** the structure of the
      entire assembly produced in step (iii). The locked rotation and
      translation functions simplify the structure-determination process in the
presence
      of NCS. Instead of searching for each monomer sep., the locked calcns.
      search for a single rotation or translation. Moreover, the locked
      functions reduce the noise level in the calcn., owing to the averaging
      over the NCS elements, and increase the signals as all monomers of the
      assembly are taken into account at the same time.
RE.CNT 13   THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2   ANSWER 24 OF 71 CAPLUS COPYRIGHT 2004 ACS on STN
AN   2000:847724 CAPLUS
DN   134:128180
TI   An approach to multi-copy search in **molecular**
      replacement
AU   Vagin, Alexei; Teplyakov, Alexei
CS   Department of Chemistry, University of York, Heslington, York, YO1 5DD, UK
SO   Acta Crystallographica, Section D: Biological Crystallography (2000),
      D56(12), 1622-1624

PB   Munksgaard International Publishers Ltd.
DT   Journal
LA   English
AB   The **mol.-replacement** method has been extended to a
      simultaneous search for multiple copies of the macromol. in the unit cell.
      The central point of this approach is the construction of a multi-copy
      search model from the properly oriented monomers using a
      special translation function. The multi-copy search method has been
      implemented in the program MOLREP and successfully tested using exptl.
      data.
RE.CNT 15   THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2   ANSWER 25 OF 71   CAPLUS   COPYRIGHT 2004 ACS on STN
AN   2000:807192   CAPLUS
DN   134:112341
TI   Does NMR Mean "Not for **Molecular Replacement**"? Using
      NMR-Based **Search Models** to Solve **Protein**
      Crystal Structures
AU   Chen, Y. W.; Dodson, E. J.; Kleywegt, G. J.
CS   Centre for Protein Engineering and Cambridge University Chemical
      Laboratory, MRC Centre, Cambridge, CB2 2QH, UK
SO   Structure (London) (2000), 8(11), R213-R220
      CODEN: STRUE6; ISSN: 0969-2126
PB   Elsevier Science Ltd.
DT   Journal; General Review
LA   English
AB   A review with 47 refs. The test cases discussed in this study show that
      using NMR models to search for MR solns. is now quite feasible, at least
      in favorable circumstances. Modern NMR studies now provide models which
      are more similar to those found by crystallog. techniques, indicating that
      the protein folds found in the solution usually closely resemble those in the
      crystal and helping to scotch the belief that the crystal environment
      distorts the protein. Techniques developed for utilizing NMR models
      should be valid for performing MR studies with distantly homologous
      proteins. This could prove to be a valuable tool for structural genomics.
      However, MR techniques still do not guarantee success and further studies
      are required to fully exploit this method.
RE.CNT 47   THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib,kwic 11-22

L3   ANSWER 11 OF 22 WPIDS COPYRIGHT 2004 THOMSON DERWENT on STN
AN   2003-403195 [38]   WPIDS
DNN   N2003-321578   DNC C2003-107403
TI   New S8 protein defined from Staphylococcus aureus, useful for identifying
      inhibitors of the rRNA-binding activity of S. aureus S8, and in screening
      of molecules and/or designing of new molecules that bind to the S8 protein
      structure.
DC   B04 D16 S03 T01
IN   CONCHA, N O; GONTAREK, R R; JANSON, C A
PA   (SMIK) SMITHKLINE BEECHAM CORP
CYC   101 .
PI   WO 2003033531   A1 20030424 (200338)* EN   41
        RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR IE IT KE LS LU
            MC MW MZ NL OA PT SD SE SK SL SZ TR TZ UG ZM ZW
         W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
            DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
            KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
            RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VC VN YU ZA
            ZM ZW
ADT   WO 2003033531 A1 WO 2002-US32859 20021015
PRAI US 2001-329439P   20011015
AB   . . .
      a protein having the coordinates listed in the specification;
          (2) a heavy atom derivative of a S. aureus S8 **protein**
      crystal, where the rRNA-binding function comprises a protein
      having the coordinates listed in the specification;
          (3) a process for identifying an. . . crystal or its portions, to
      determine a crystal form of a mutant, homolog or co-complex of the
      rRNA-binding function by **molecular replacement**;
          (6) a process for designing drugs for inhibiting S. aureus S8
      activity using the atomic coordinates of a S. aureus. . . .
TECH. . .
      of S8 lined by residues 4-6, 30-32, 56-57, 82-92, 107-111, and 122-125
      that interact with nucleotides A587-A758. The S8 rRNA-binding
      protein in **crystalline** form has lattice constants of a =
      42.1Angstrom, b = 55.9Angstrom, c = 61.3Angstrom, alpha = 09.0degrees,
      beta = 09.0degrees,. . .

L3   ANSWER 12 OF 22 WPIDS COPYRIGHT 2004 THOMSON DERWENT on STN
AN   2003-247867 [24]   WPIDS
DNC   C2003-063733
TI   Novel 2C-methyl-D-erythritol 2,4-cyclodiphosphate synthase protein or its
      functional **protein** subunit, in **crystalline** form,
      useful for identifying and designing inhibitors and activators of the
      protein.
DC   B04 C06 D16
IN   BUCHANAN, S G; GAJIWALA, K S; LOUIE, G V; SAUDER, J M; SAUDER, M J
PA   (STRU-N) STRUCTURAL GENOMIX; (BUCH-I) BUCHANAN S G; (GAJI-I) GAJIWALA K S;
      (LOUI-I) LOUIE G V; (SAUD-I) SAUDER J M; (STRU-N) STRUCTURAL GENOMIX INC
CYC   100
PI   WO 2002102991   A2 20021227 (200324)* EN   370
        RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
            NL OA PT SD SE SL SZ TR TZ UG ZM ZW
         W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
            DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
            KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
            RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM
            ZW

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        US 2003073134   A1 20030417 (200329)
        AU 2002322265   A1 20030102 (200452)
ADT     WO 2002102991 A2 WO 2002-US19451 20020617; US 2003073134 A1 Provisional US
        2001-299058P 20010618, US 2002-174410 20020617; AU 2002322265 A1 AU
        2002-322265 20020617
FDT     AU 2002322265 A1 Based on WO 2002102991
PRAI    US 2001-299058P        20010618; US 2002-174410       20020617
TI      Novel 2C-methyl-D-erythritol 2,4-cyclodiphosphate synthase protein or its
        functional protein subunit, in crystalline form,
        useful for identifying and designing inhibitors and activators of the
        protein.
AB      WO2002102991   UPAB: 20030410
        NOVELTY - A 2C-methyl-D-erythritol 2,4-cyclodiphosphate synthase (MECPS)
        protein (I) or a functional MECPS protein subunit, in
        crystalline form, is new.
              DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the
        following:
              (1) Producing (M1) a.  .  .
TECH.   .  .
        binding pocket of a MECPS protein, by obtaining 3D structural coordinates
        defining the protein or a binding pocket of the protein, from a
        crystal of the protein; and
        (b) introducing the structural coordinate into a computer to produce a
        database containing the molecular structural coordinates of the protein or
        binding pocket.
        M2 comprises:
        (a) generating a representation of binding pocket of a MECPS
        protein in a co-crystal with a compound, preferably a
        compound rationally designed to be capable of binding the binding pocket
        by preparing a binding.  .  .  MECPS active site or binding pocket; and
        (c) determining whether the potential modulator activates or inhibits the
        activity of the protein.
        M5 comprises:
        (a) generating an X-ray diffraction pattern from a
        crystallized form of the molecule or molecular complex, using a
        molecular replacement method to interpret the structure
        of the molecule, where the molecular replacement
        method uses the structural coordinates given in the specification, or its
        subset comprising a binding pocket, where the structural coordinates.  .
        .
TT      TT: NOVEL METHYL ERYTHRITOL SYNTHASE PROTEIN FUNCTION
        PROTEIN CRYSTAL FORM USEFUL IDENTIFY DESIGN INHIBIT
        ACTIVATE PROTEIN.


L3      ANSWER 13 OF 22   WPIDS   COPYRIGHT 2004 THOMSON DERWENT on STN
AN      2003-247844 [24]    WPIDS
DNN     N2003-197048        DNC C2003-063714
TI      New pyrazolo(3,4-c)pyridazine derivatives are glucogen synthase kinase -3
        inhibitors useful for treating e.g. schizophrenia, Alzheimer's disease,
        diabetes, autoimmune diseases, allergy, asthma, multiple sclerosis, and
        baldness.
DC      B02 B04 S03 T01
IN      ARNOST, M J; GREEN, J; HAAR, E T; SWENSON, L; TER HAAR, E
PA      (ARNO-I) ARNOST M J; (GREE-I) GREEN J; (HAAR-I) HAAR E T; (SWEN-I) SWENSON
        L; (VERT-N) VERTEX PHARM INC
CYC     101
PI      WO 2002088078   A2 20021107 (200324)* EN   778
            RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
                NL OA PT SD SE SL SZ TR TZ UG ZM ZW
             W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
                DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
                KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
                RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM
                ZW
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      US 2003125332    A1 20030703 (200345)
      AU 2002259071    A1 20021111 (200433)
      EP 1435957       A2 20040714 (200446)   EN
          R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT
             RO SE SI TR
ADT   WO 2002088078 A2 WO 2002-US13511 20020429; US 2003125332 A1 Provisional US
      2001-287366P 20010430, Provisional US 2001-297094P 20010608, Provisional
      US 2002-361899P 20020227, US 2002-135255 20020429; AU 2002259071 A1 AU
      2002-259071 20020429; EP 1435957 A2 EP 2002-729056 20020429, WO
      2002-US13511 20020429
FDT   AU 2002259071 A1 Based on WO 2002088078; EP 1435957 A2 Based on WO
      2002088078
PRAI  US 2002-361899P     20020227; US 2001-287366P      20010430;
      US 2001-297094P     20010608; US 2002-135255        20020429
AB    .  .  .
      complex comprising (C2) involves:
           (i) producing and purifying GSK-3 beta protein;
           (ii) mixing a crystallization solution with the protein
      complex to produce a crystallizable composition; and
           (iii) crystallizing the composition;
           (4) A molecule or molecular complex comprises a binding pocket
      defined by.  .  .
TECH.    .  .
      a display terminal, a printer or disk drive.

      TECHNOLOGY FOCUS - BIOLOGY - Preferred Components: (C2) is HSSPHQpSEDEEE.
      The GSK-3beta protein in the crystal is selected from
      420 amino acid sequences as given in the specification, amino acid
      residues 7 - 420 of the.  .  .

L3    ANSWER 14 OF 22  WPIDS  COPYRIGHT 2004 THOMSON DERWENT on STN
AN    2003-229481 [22]    WPIDS
CR    2003-221757 [21]
DNN   N2003-182547        DNC C2003-059031
TI    Novel perosamine synthase homolog protein or its functional
      protein subunit, in a crystalline form, useful for
      identifying and designing inhibitors and activators of the protein, and
      for designing antimicrobials.
DC    B04 D16 T01
IN    BADGER, J; BUCHANAN, S G; HANS-JOACHIM, M; HENDLE, J; NOLAND, B;
      MULLER-DIECKMANN, H
PA    (BADG-I) BADGER J; (BUCH-I) BUCHANAN S G; (HEND-I) HENDLE J; (MULL-I)
      MULLER-DIECKMANN H; (NOLA-I) NOLAND B; (STRU-N) STRUCTURAL GENOMIX INC
CYC   100
PI    WO 2003006617    A2 20030123 (200322)* EN   424
          RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR IE IT KE LS LU
              MC MW MZ NL OA PT SD SE SK SL SZ TR TZ UG ZM ZW
           W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
              DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
              KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
              RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM
              ZW
      US 2003101005    A1 20030529 (200337)
      AU 2002332410    A1 20030129 (200452)
ADT   WO 2003006617 A2 WO 2002-US21935 20020712; US 2003101005 A1 Provisional US
      2001-305428P 20010713, US 2002-194728 20020712; AU 2002332410 A1 AU
      2002-332410 20020712
FDT   AU 2002332410 A1 Based on WO 2003006617
PRAI  US 2001-305428P     20010713; US 2002-194728        20020712
TI    Novel perosamine synthase homolog protein or its functional
      protein subunit, in a crystalline form, useful for
      identifying and designing inhibitors and activators of the protein, and
      for designing antimicrobials.
AB    WO2003006617   UPAB: 20040813
```

NOVELTY - An perosamine synthase homolog (PSH) protein (I), or a
functional subunit of PSH **protein**, in its **crystalline**
form, is new.
     DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the
following:
     (1) producing (M1) a. . . pocket of a PSH protein, by:
     (a) obtaining 3D structural coordinates defining the protein or a
binding pocket of the **protein**, from a **crystal** of the
protein; and
     (b) introducing the structural coordinate into a computer to produce
a database containing the molecular. . . produced by M1;
     (3) producing (M2) a computer readable database comprising a
representation of a binding pocket of a PSH **protein** in a co-
crystal with a compound, optionally with a compound rationally
designed to be capable of binding a binding pocket of a PSH. . .
unknown structure, by generating an X-ray diffraction pattern from a
crystallized form of the molecule or molecular complex, using a
molecular replacement method to interpret the structure
of the molecule, where the **molecular replacement**
method uses the structural coordinates given in the specification, or its
subset comprising a binding pocket, where the structural coordinates. .
.

TT   TT: NOVEL SYNTHASE HOMOLOGUE **PROTEIN** FUNCTION **PROTEIN**
     CRYSTAL FORM USEFUL IDENTIFY DESIGN INHIBIT ACTIVATE PROTEIN
     DESIGN ANTIMICROBIAL.

L3   ANSWER 15 OF 22 WPIDS COPYRIGHT 2004 THOMSON DERWENT on STN
AN   2003-221757 [21]   WPIDS
CR   2003-229481 [22]
DNC C2003-056524
TI   Novel AmB amino transferase protein or its functional **protein**
     subunit, in a **crystalline** form, useful for identifying and
     designing inhibitors and activators of the protein, and for designing
     antimicrobials.
DC   B04 D16
IN   BADGER, J; BUCHANAN, S G; HENDLE, J; NEWMAN, J; NOLAND, B
PA   (BADG-I) BADGER J; (BUCH-I) BUCHANAN S G; (HEND-I) HENDLE J; (NEWM-I)
     NEWMAN J; (NOLA-I) NOLAND B; (STRU-N) STRUCTURAL GENOMIX INC
CYC 100
PI   WO 2003006674   A2 20030123 (200321)* EN 289
     RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR IE IT KE LS LU
        MC MW MZ NL OA PT SD SE SK SL SZ TR TZ UG ZM ZW
      W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
        DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
        KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
        RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM
        ZW
     US 2003105010   A1 20030605 (200339)
     AU 2002322445   A1 20030129 (200452)
ADT WO 2003006674 A2 WO 2002-US21937 20020712; US 2003105010 A1 Provisional US
     2001-305428P 20010713, US 2002-193858 20020712; AU 2002322445 A1 AU
     2002-322445 20020712
FDT AU 2002322445 A1 Based on WO 2003006674
PRAI US 2001-305428P   20010713; US 2002-193858   20020712
TI   Novel AmB amino transferase protein or its functional **protein**
     subunit, in a **crystalline** form, useful for identifying and
     designing inhibitors and activators of the protein, and for designing
     antimicrobials.
AB   WO2003006674   UPAB: 20040813
     NOVELTY - An AmB aminotransferase (AmB) protein (I), or a functional
     subunit of AmB **protein**, in its **crystalline** form, is
     new.
        DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the
     following:

(1) producing (M1) a computer. . . binding pocket of a AmB
protein, by obtaining 3D structural coordinates defining the protein or a
binding pocket of the **protein,** from a **crystal** of the
protein, and introducing the structural coordinate into a computer to
produce a database containing the molecular structural coordinates. . .
produced by M1;
        (3) producing (M2) a computer readable database comprising a
representation of a binding pocket of a AmB **protein** in a co-
crystal with a compound, optionally with a compound rationally
designed to be capable of binding a binding pocket of a AmB. . .
unknown structure, by generating an X-ray diffraction pattern from a
crystallized form of the molecule or molecular complex, using a
molecular replacement method to interpret the structure
of the molecule, where the **molecular replacement**
method uses the structural coordinates given in the specification, or its
subset comprising a binding pocket, where the structural coordinates. .
.

TT   TT: NOVEL AMINO TRANSFERASE **PROTEIN** FUNCTION **PROTEIN**
        CRYSTAL FORM USEFUL IDENTIFY DESIGN INHIBIT ACTIVATE PROTEIN
        DESIGN ANTIMICROBIAL.

L3   ANSWER 16 OF 22   WPIDS   COPYRIGHT 2004 THOMSON DERWENT on STN
AN   2003-112007 [10]   WPIDS
DNN   N2003-089147   DNC C2003-028697
TI   Identifying a search model to use in **molecular**
      replacement for determining a structure of a target biomolecule
      from crystal data comprises employing computer executable logic.
DC   B04 D16 T01
IN   ABOLA, E; DAVID, P R; DELFT, F V; MCREE, D; RAMMELKAMP, J; VON DELFT, F
PA   (ABOL-I) ABOLA E; (DAVI-I) DAVID P R; (DELF-I) DELFT F V; (MCRE-I) MCREE
      D; (RAMM-I) RAMMELKAMP J; (SYRR-N) SYRRX INC
CYC   100
PI   WO 2002091287   A2 20021114 (200310)* EN   58
        RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
            NL OA PT SD SE SL SZ TR TZ UG ZM ZW
        W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
           DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR
           KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT
           RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM
           ZW
      US 2002183861   A1 20021205 (200310)
      AU 2002305345   A1 20021118 (200452)
ADT   WO 2002091287 A2 WO 2002-US13988 20020503; US 2002183861 A1 US 2001-848866
      20010504; AU 2002305345 A1 AU 2002-305345 20020503
FDT   AU 2002305345 A1 Based on WO 2002091287
PRAI US 2001-848866   20010504
TI   Identifying a search model to use in **molecular**
      replacement for determining a structure of a target biomolecule
      from crystal data comprises employing computer executable logic.
AB   WO 200291287   UPAB: 20030211
      NOVELTY - Identifying a search model to use in **molecular**
      replacement for determining a structure of a target biomolecule
      from crystal data comprises employing computer executable logic.
        DETAILED DESCRIPTION - Identifying a search model to use in
      molecular replacement for determining a structure of a
      target biomolecule from crystal data comprises:
        (a) employing computer executable logic to perform multiple
      molecular replacement searches on crystal data of the
      target biomolecule, where a group of different biomolecule structures are
      used as search models for the multiple **molecular**
      replacement searches; and
        (b) employing computer executable logic to compare solutions from the
      multiple **molecular replacement** searches, where the
      comparison produces data from which biomolecule structures in the group

can be identified as having superior structural. . . medium, useful in association with a computer that includes a processor and a memory, comprising:
        (a) logic for performing multiple **molecular replacement** searches on crystal data or diffraction data of a target biomolecule where a group of different biomolecule structures are used as search models for the multiple **molecular replacement** searches; and
        (b) logic for comparing solutions from the multiple **molecular replacement** searches.
        USE - The method is useful for identifying a search model in **molecular replacement** for determining a structure of a target biomolecule from crystal data (claimed).
Dwg.0/3

TECH   UPTX: 20030211
TECHNOLOGY FOCUS - BIOTECHNOLOGY - Preferred Method: Identifying a search model for use in **molecular replacement** for determining a structure of a target biomolecule from crystal data further comprises employing computer executable logic to select the. . . structures used to perform the multiple replacement searches. The biomolecule is a protein, DNA, RNA or a complex comprising a **protein,** DNA or RNA. The **crystal** data is X-ray diffraction data, neutron diffraction crystal data, magnetic crystal data, nuclear magnetic resonance crystal data or mass spectrometry crystal data. **Molecular replacement** is performed using a program comprising AmoRe, BRUTE, COMO (Combined **molecular replacement**) , CNS (Crystallography and NMR System), TNT, GLRF (General locked rotation function program), TRANSF (Translation function program), TF (translation function. . . (Fourier inversion direct to reciprocal space) program) or FFTEXP (Reflection data expanding program), preferably EPMR (a program that finds crystallographic **molecular replacement** solutions using an evolutionary search algorithm), or a **molecular replacement** program comprising an evolutionary algorithm for searching six-dimensional space.
Comparing **molecular replacement** solutions comprises:
(a) comparing figures of merit calculated for the **molecular replacement** solutions;
(b) performing a statistical analysis on figures of merit calculated for the **molecular replacement** solutions;
(c) determining which of the biomolecule structures in the group produced a **molecular replacement** solution whose figure of merit is at least two, three, five or ten standard deviations better than the average figure of merit for **molecular replacement** solutions for the biomolecule structures in the group;
(d) comparing root mean square errors for each **molecular replacement** solution of a probability-weighted average over all possible phase choices;
(e) establishing a background correlation level between the biomolecule structures in the group and the target biomolecule based on the **molecular replacement** solutions and determining which of the biomolecule structures in the group produced a **molecular replacement** solution that exceeds the background correlation level by at least two, three, five or ten standard deviations.
The group of different biomolecule structures on which **molecular replacement** searches are performed comprises:
(a) at least 3 different biomolecule structures, at least one biomolecule structure that has less than. . . comprises a combination of two or more structure fragments. The data produced from the comparison identifies which biomolecule structures produced **molecular replacement** solutions that are at least among the top 35% of **molecular replacement** solutions produced by the group, or that are at least 2, 3, 5 or ten standard deviations better than the **molecular replacement** solutions produced by the group.
Selection of the group of biomolecule structures is:

(a) based, at least in part, on sequence. . . iterative.
Selection of the members of the group of biomolecule structures is
performed until a biomolecule structure is selected whose
molecular replacement solution is at least 2, 3, 5 or
ten standard deviations better than the **molecular
replacement** solution for the biomolecule structures in the group.